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STRUCTURES OF METALLOCARBORANES. IX. CRYSTAL AND MOLECULAR STRU--ETC(U)  
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Crystal and Molecular Structure of the Ten-Vertex Heterobimetallocarborane 2,

3-Di-<sup>eta</sup>-cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8),

2,3-( $\eta$ -C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>-(2,3)-NiCo-10-CB<sub>7</sub>H<sub>8</sub>.

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10 G. E. Hardy, K. P. Callahan, M. F. Hawthorne

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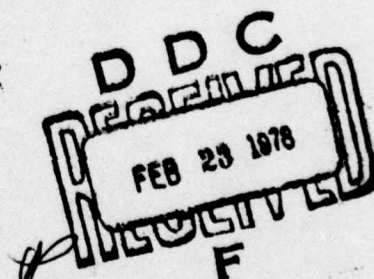
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$2,3-(\eta\text{-C}_5\text{H}_5)_2\text{-(2,3)-NiCo-10-CB}_7\text{H}_8^1$

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### ABSTRACT

A complete three dimensional crystal structure determination of the title compound was carried out. Crystal data: Space group C2/c,  $a = 15.794(4)$ ,  $b = 7.955(2)$ ,  $c = 24.273(7)$  Å,  $\beta = 104.12(2)^\circ$ ,  $z = 8$ ,  $d_o = 1.55(2)$ ,  $d_c = 1.54$ . Diffraction data to  $2\theta_{\max} = 50^\circ$  were obtained with a Syntex P1 automated diffractometer (MoK $_{\alpha}$  radiation) and the structure was solved by conventional Patterson, Fourier and full matrix least-squares techniques to a conventional  $R = 0.047$  for 2048 independent non-zero reflections. The molecule has the bicapped square antiprismatic geometry expected for a closo ten-vertex polyhedron. The two metal atoms are indistinguishable and occupy adjacent sites in the same equatorial belt. The carbon atom resides in the four-coordinate site non-adjacent to the two metal atoms.



## INTRODUCTION

Polyhedral expansion of the monocarbacobaltacarborane anion  $[\text{C}_5\text{H}_5\text{Co-CB}_7\text{H}_8]^-$  with  $\text{NiBr}_2 \cdot 2 \text{ glyme}$  in the presence of  $\text{C}_5\text{H}_5^+$  affords several neutral isomeric complexes of the formula  $(\text{C}_5\text{H}_5)_2\text{NiCoCB}_7\text{H}_8$  which contain formal Ni(IV) and Co(III) vertices, and which are isoelectronic with  $(\text{C}_5\text{H}_5)_2\text{Co}_2\text{C}_2\text{B}_6\text{H}_8$ . The structure of one isomer of the latter has previously been reported; the mixed cobalt-nickel compounds exist in more numerous isomeric forms. An x-ray structural investigation of one isomer of this complex is reported herein.

## UNIT CELL AND SPACE GROUP

A sample of the compound was furnished by Dr. C. G. Salentine. It was found to be stable to both air and x-rays. Preliminary x-ray diffraction photographs of the black crystals indicated monoclinic symmetry with systematic absences indicative of space groups  $\text{C}2/c$  or  $\text{Cc}$ . The density, measured by flotation, was  $1.55(2) \text{ g cm}^{-3}$ , in good agreement with the calculated density of  $1.54 (z = 8)$ .

## COLLECTION AND REFINEMENT OF X-RAY DATA

Intensity data were collected on a Syntex PT automated diffractometer equipped with scintillation counter and pulse height analyzer. A graphite crystal was used to produce monochromatic  $\text{MoK}_\alpha$  radiation ( $\lambda = 0.71069 \text{ \AA}$ ). Fifteen automatically centered reflections were used in the determination of the lattice parameters;  $a = 15.794(4) \text{ \AA}$ ,  $b = 7.955(2) \text{ \AA}$ ,  $c = 24.273(7) \text{ \AA}$ ,  $\beta = 104.12(2)^\circ$ . Intensity data were collected on a small crystal of irregular shape (average diameter about  $0.1 \text{ mm}$ ) with a  $\theta$ - $2\theta$  scan technique to a limit of  $2\theta = 50^\circ$ . Reflections were scanned at a constant rate of  $2.0^\circ/\text{min}$  from  $1^\circ$  below the

$K_{\alpha 1}$  reflection to  $1.0^\circ$  above the  $K_{\alpha 2}$  reflection. Background was measured at each end of the scan. The total time counting background was equal to the scan time for each reflection. The intensities of three standard reflections were measured after every 97 reflections. No significant change in the intensities of these reflections was observed in the course of the data collection.

The reflections were corrected for Lorentz and polarization effects. The intensity of a reflection,  $I(hkl)$ , and  $\sigma[I(hkl)]$ , its estimated standard deviation, were calculated according to the equations  $I = CT - (t_c/t_b)(B1+B2)/2$  and  $\sigma = \{\sigma_s^2 + [(0.04I)^2]\}^{1/2}$ , where  $I$  is the net integrated intensity,  $CT$  is the total integrated count,  $t_c$  and  $t_b$  are the times employed for counting the scan and background, respectively,  $B1$  and  $B2$  are the background counts on the low and high sides of the reflection, and  $\sigma_s$  is the standard deviation in the intensity due to counting statistics. Reflections having intensities less than three times their standard deviations were defined as unobserved and not included in subsequent calculations. Because of the small and irregular shape of the crystal, no absorption correction was applied.

#### SOLUTION AND REFINEMENT OF THE STRUCTURE

The coordinates of the two metal atoms were determined by the solution of a three-dimensional Patterson map, and a Fourier map based on these positions revealed the positions of all the non-hydrogen cage atoms. Successive Fourier maps were used to identify the positions of the cyclopentadienyl carbon atoms. Full matrix least-squares refinement of these parameters was followed by a Fourier difference map in which all the cage hydrogen atoms except H9 were located. Idealized positions for the cyclopentadienyl hydrogen atoms and for H9 were calculated, and the position of all hydrogen atoms were refined in subsequent least-squares cycles. The position of the carbon atom was identified by short bond distances to its neighbors and its small temperature factor when



refined as a boron atom. No distinction could be made between the two metal sites and therefore they were both assigned scattering factors which corresponded to the average of the nickel and cobalt scattering factors. In the final refinement, the positions of all atoms and anisotropic thermal parameters for all non-hydrogen atoms were refined. The temperature factors for the hydrogen atoms were set at 2.0. This refinement converged to  $R = 4.7\%$ .

The programs used in this structure determination, the scattering factors and the refinement techniques, were the same as those used in the preceding paper.<sup>1</sup>

The final observed atomic fractional coordinates are collected in Table I. Anisotropic thermal parameters are presented in Table II. The final observed calculated structure factors are available.<sup>7</sup>

#### THE MOLECULAR STRUCTURE AND DISCUSSION

Intramolecular distances and their estimated standard deviations (esd's) are listed in Table IIIa. Average bond distances, with their root-mean-square deviations, are collected in Table IIIb. The individual bond angles and their associated esd's are presented in Table IV. The structure of  $(C_5H_5)_2NiCoCB_7H_8$  is shown in Figure 1, which also illustrates the numbering system employed.<sup>8</sup>

The structure of the complex may be described as a distorted bicapped square antiprism, a 10-vertex closed polyhedron comprised of seven boron, one carbon, one cobalt, and one nickel atom vertices. The carbon and boron atoms are further bonded to terminal hydrogen atoms, while the metal vertices are attached to  $\eta$ -cyclopentadienyl ligands. The metals occupy adjacent equatorial positions on the polyhedral framework,  $2.4492(11)\text{\AA}$  apart, while the apical positions are occupied by one boron atom and the carbon atom. The metals reside in the same equatorial belt, the belt closest to the apical boron atom and furthest removed from the apical carbon atom. The positions occupied by the metals are totally equivalent in the polyhedron, and there is consequent



random orientation of the two metals such that specification of the unique positions of the cobalt or nickel vertices is impossible. Instead, an averaged "half-nickel, half-cobalt" atom is seen at those two sites. The polyhedron exhibits mirror symmetry; the mirror plane, which includes atoms B1, B6, B8 and C10, is not crystallographically required but related bond distances are equal within three standard deviations.

This compound is a close analog of the bimetallocarborane  $(C_5H_5)_2Co_2C_2B_6H_8$ , whose structure has been previously reported.<sup>6</sup> This latter species has the same overall geometry, with the two cobalt atoms occupying different equatorial belts, (still in adjacent polyhedral positions at a distance of  $2.489(1)\overset{0}{\text{\AA}}$ ) and the two carbon atoms at the two low-coordinate apical positions. Rationalizations of the energetic relationship between these two geometries are complicated by the observation that while  $(C_5H_5)Co_2C_2B_6H_8$  thermally rearranges to give an isomer with non-adjacent metal vertices, the isomer of  $(C_5H_5)CoNiCB_7H_8$  studied here is stable to thermal rearrangement at  $450^\circ\text{C}$ . Both  $(C_5H_5)_2Co_2C_2B_6H_8$  and  $(C_5H_5)_2NiCoCB_7H_8$  fit the theoretical models of closo-metallocarboranes<sup>9</sup> in that they are constituted of  $n = 10$  polyhedral atoms and  $2n + 2$  electron pairs or 22 framework electrons. Another 10-vertex complex  $(C_5H_5)_2Fe_2C_2B_6H_8$ , whose structure was recently reported,<sup>10</sup> is two electrons short of the  $2n + 2$  rule and exhibits major distortion from the idealized closo structure of a bicapped square antiprism. The symmetrical structure and lack of distortion (other than that produced by the presence of heteroatoms) found for  $(C_5H_5)_2NiCoCB_7H_8$  is good evidence for the validity of the electron-counting scheme and lends further justification to the idea previously put forth<sup>9,11</sup> that  $\{C_5H_5Co\}$  is electronically equivalent to  $\{BH\}$  and that  $\{C_5H_5Ni\}$  is equivalent to a polyhedral  $\{CH\}$  group, for similar geometries are observed in the electronically similar complexes  $(C_5H_5)_2NiCoCB_7H_8$ ,  $(C_5H_5)_2Co_2C_2B_6H_8$ ,<sup>6</sup>  $(CoC_2B_7H_9)_2^-$ ,<sup>12</sup>  $C_2B_8H_{10}$ ,<sup>13</sup>

and  $B_{10}H_{10}^{2-}$ .<sup>14</sup> Within experimental errors, all equivalent bond distances are the same in this series of compounds.<sup>15</sup>

Although it is impossible to discern between the cobalt and nickel atoms, it is interesting that the metal-metal distance is significantly shorter than is the Co-Co distance in  $(C_5H_5)_2Co_2C_2B_6H_8$ . It should be noted that "tropical"<sup>12</sup> bond distances in bicapped square antiprisms are generally found to be longer than "equatorial" bond distances, thus diminishing the significance of this observation.

The cyclopentadienyl rings, while exhibiting the large librational motion typical in compounds of this type studied at room temperature, exhibit  $D_{5h}$  symmetry, as expected. The metal-carbon distances to the cyclopentadienyl rings are again equal within experimental error, further establishing the positional disorder of the metals.

#### Acknowledgments

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Supplementary Material available.<sup>7</sup>



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15. See Reference 6 for a compilation.



TABLE I

Final Atomic Parameters<sup>a</sup>

<u>Atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
M2	0.21175(4)	0.61403(10)	0.36659(3)
M3	0.36816(4)	0.61233(10)	0.37044(3)
B1	0.2730(5)	0.4860(9)	0.3172(3)
B4	0.3455(6)	0.3492(9)	0.3619(3)
B5	0.2289(5)	0.3506(9)	0.3579(4)
B6	0.3133(4)	0.5962(0)	0.4404(3)
B7	0.3931(5)	0.4177(9)	0.4308(3)
B8	0.3051(6)	0.2697(10)	0.4187(4)
B9	0.2243(5)	0.4215(9)	0.4277(3)
C10	0.3208(4)	0.4129(8)	0.4664(3)
Cp1	0.1722(6)	0.8495(11)	0.3364(8)
Cp2	0.1257(9)	0.7368(22)	0.3024(4)
Cp3	0.0813(7)	0.6434(13)	0.3329(9)
Cp4	0.1046(7)	0.7121(22)	0.3873(8)
Cp5	0.1588(10)	0.8352(19)	0.3871(5)
Cp6	0.4948(7)	0.6750(23)	0.3805(11)
Cp7	0.4573(15)	0.7959(29)	0.4011(6)
Cp8	0.3984(9)	0.8544(12)	0.3577(13)
Cp9	0.3995(11)	0.7682(31)	0.3113(6)
Cp10	0.4608(14)	0.6562(18)	0.3272(11)
CpH1	0.211(4)	0.921(7)	0.334(3)
CpH2	0.129(4)	0.735(8)	0.271(3)
CpH3	0.049(4)	0.561(7)	0.328(3)
CpH4	0.085(4)	0.679(8)	0.412(3)
CpH5	0.174(4)	0.880(9)	0.413(3)
CpH6	0.523(4)	0.618(8)	0.399(3)
CpH7	0.473(4)	0.820(8)	0.429(3)
CpH8	0.365(4)	0.917(7)	0.352(3)
CpH9	0.368(4)	0.771(7)	0.277(3)

Table I. Final Atomic Parameters (cont'd)

<u>Atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
CpH10	0.473(4)	0.594(7)	0.309(3)
B1H	0.259(3)	0.494(7)	0.272(2)
B4H	0.375(4)	0.293(7)	0.335(2)
B5H	0.181(3)	0.275(7)	0.337(2)
B6H	0.320(3)	0.690(7)	0.468(2)
B7H	0.454(4)	0.412(7)	0.449(2)
B8H	0.306(3)	0.137(6)	0.432(2)
B9H	0.164(4)	0.390(7)	0.444(2)
C10H	0.334(4)	0.387(7)	0.506(2)

<sup>a</sup>Values in parentheses are estimated standard deviations and refer to the last digit of the preceding number.

TABLE II

Anisotropic Thermal Parameters  $\times 10^4$ <sup>a</sup>

<u>Atom</u>	<u>B<sub>11</sub></u>	<u>B<sub>22</sub></u>	<u>B<sub>33</sub></u>	<u>B<sub>12</sub></u>	<u>B<sub>13</sub></u>	<u>B<sub>23</sub></u>
M2	27.2(4)	117.2(15)	12.8(2)	-4.3(6)	5.6(2)	5.1(4)
M3	27.5(4)	113.7(15)	14.9(2)	3.0(6)	5.9(2)	5.4(5)
B1	46(4)	149(13)	12.1(13)	-20(6)	3.6(17)	-11(4)
B4	69(5)	101(14)	21(2)	16(6)	15(2)	-11(4)
B5	57(4)	114(15)	21(2)	-31(6)	6(2)	-8(4)
B6	50(4)	155(14)	9.6(12)	4(6)	3.7(16)	-6(4)
B7	45(4)	131(15)	17.2(16)	13(6)	4.7(19)	6(4)
B8	66(5)	125(14)	23(2)	-5(6)	12(2)	12(4)
B9	58(4)	127(15)	19(2)	-13(6)	8(2)	16(4)
C10	64(4)	171(14)	15.1(13)	9(5)	7.7(17)	12(4)
Cp1	37(4)	169(17)	64(5)	31(6)	20(4)	53(7)
Cp2	84(7)	485(36)	17(2)	118(13)	5(3)	45(8)
Cp3	42(5)	215(23)	65(5)	-25(8)	-23(5)	9(9)
Cp4	48(6)	459(38)	57(6)	92(12)	42(5)	102(13)
Cp5	92(10)	301(37)	33(3)	107(16)	7(4)	-25(7)
Cp6	32(4)	493(45)	78(7)	1(11)	-4(5)	129(14)
Cp7	125(11)	540(42)	38(3)	-207(18)	35(5)	-62(11)
Cp8	51(6)	112(18)	115(9)	11(7)	43(6)	55(10)
Cp9	82(9)	588(51)	30(3)	130(18)	-8(4)	89(10)
Cp10	116(11)	333(36)	74(6)	-52(16)	79(7)	-44(12)

<sup>a</sup>See footnote a of Table I. The anisotropic temperature factor  $T$  is defined as  $T = \exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl)]$ . Thermal ellipsoids are depicted in the figure.



TABLE IIIa

Interatomic Distances<sup>a</sup>

<u>Atoms</u>	<u>Distance, Å</u>	<u>Atoms</u>	<u>Distance, Å</u>
I. Distances around Metal Atoms			
M2-M3	2.4492(11)	M3-Cp6	2.018(10)
M2-Cp1	2.052(8)	M3-Cp7	2.040(9)
M2-Cp2	2.049(7)	M3-Cp8	2.027(8)
M2-Cp3	2.037(9)	M3-Cp9	2.048(10)
M2-Cp4	2.034(10)	M3-Cp10	2.028(10)
M2-Cp5	2.060(9)	M3-B1	1.998(6)
M2-B1	1.993(8)	M3-B4	2.126(7)
M2-B5	2.129(7)	M3-B6	2.090(8)
M2-B6	2.097(6)	M3-B7	2.102(7)
M2-B9	2.109(7)		
II. Distances in Cyclopentadienyl Rings			
Cp1-Cp2	1.315(15)	Cp6-Cp7	1.293(19)
Cp1-Cp5	1.304(15)	Cp6-Cp10	1.281(19)
Cp2-Cp3	1.360(17)	Cp7-Cp8	1.310(18)
Cp3-Cp4	1.393(18)	Cp8-Cp9	1.322(20)
Cp4-Cp5	1.302(17)	Cp9-Cp10	1.303(18)
III. Boron-Boron Distances			
B1-B4	1.750(10)	B5-B9	1.803(13)
B1-B5	1.720(11)	B6-B7	1.949(10)
B4-B5	1.820(12)	B6-B9	1.947(10)
B4-B7	1.745(11)	B7-B8	1.790(11)
B4-B8	1.771(13)	B8-B9	1.808(12)
B5-B8	1.781(11)		

Table IIIa. Interatomic Distances (cont'd)

IV. Boron-Carbon Distances

B6-C10	1.582(9)	B8-C10	1.600(11)
B7-C10	1.591(11)	B9-C10	1.584(9)

V. Carbon-Hydrogen Distances

C10-CH10	0.95(5)	Cp6-CpH6	0.71(6)
Cp1-CpH1	0.85(6)	Cp7-CpH7	0.70(6)
Cp2-CpH2	0.79(6)	Cp8-CpH8	0.72(6)
Cp3-CpH3	0.82(6)	Cp9-CpH9	0.86(5)
Cp4-CpH4	0.78(7)	Cp10-CpH10	0.73(6)
Cp5-CpH5	0.71(6)		

VI. Boron-Hydrogen Distances

B1-BH1	1.06(5)	B7-BH7	0.96(5)
B4-BH4	0.99(6)	B8-BH8	1.10(5)
B5-BH5	1.00(5)	B9-BH9	1.15(6)
B6-BH6	1.00(5)		

<sup>a</sup>See footnote a of Table I.

TABLE IIIb

Average Bond Lengths

<u>Atoms</u>	<u>No.</u>	<u>Range<sup>a</sup>, Å</u>	<u>Average<sup>b</sup>, Å</u>
M-C	10	2.018(10)-2.060(9)	2.039(13)
M-B	8	1.993(8)-2.129(7)	2.08(5)
C-C	10	1.281(19)-1.393(18)	1.32(3)
B-B	11	1.720(11)-1.949(10)	1.81(8)
B-C	4	1.582(9)-1.600(11)	1.589(8)
C-H	11	0.70(6)-0.95(5)	0.78(8)
B-H	7	0.96(5)-1.15(6)	1.04(7)

<sup>a</sup>See footnote a of Table I. <sup>b</sup>ESD's for average bond lengths were calculated using the internal routine of an HP-45 calculator.



TABLE IV

Interatomic Angles<sup>a</sup>

<u>Atoms 1,2,3</u>	<u>Angle, Deg</u>	<u>Atoms 1,2,3</u>	<u>Angle, Deg</u>
I. Angles around Metals			
A. $C_5H_5-M-C_5H_5$			
Cp1-M2-Cp2	37.4(4)	Cp6-M3-Cp7	37.2(5)
Cp2-M2-Cp3	38.9(5)	Cp7-M3-Cp8	37.6(5)
Cp3-M2-Cp4	40.0(5)	Cp8-M3-Cp9	37.9(6)
Cp4-M2-Cp5	37.1(5)	Cp9-M3-Cp10	37.3(5)
Cp5-M2-Cp1	37.0(4)	Cp10-M3-Cp6	36.9(6)
Cp1-M2-Cp3	64.0(4)	Cp6-M3-Cp8	61.3(5)
Cp3-M2-Cp5	64.5(5)	Cp8-M3-Cp10	62.0(5)
Cp2-M2-Cp4	64.4(5)	Cp7-M3-Cp9	63.8(5)
Cp2-M2-Cp5	62.9(4)	Cp6-M3-Cp9	62.1(5)
Cp4-M2-Cp1	62.6(4)	Cp7-M3-Cp10	62.9(5)
B. $C_5H_5-M-CB_7H_8$			
Cp1-M2-B1	113.7(5)	Cp6-M3-B1	140.3(9)
Cp1-M2-B5	153.9(6)	Cp6-M3-B4	113.2(6)
Cp1-M2-B6	118.0(5)	Cp6-M3-B6	120.8(8)
Cp1-M2-B9	152.0(6)	Cp6-M3-B7	95.0(4)
Cp2-M2-B1	96.6(4)	Cp7-M3-B1	160.1(7)
Cp2-M2-B5	118.1(5)	Cp7-M3-B4	145.7(9)
Cp2-M2-B6	155.4(6)	Cp7-M3-B6	97.7(4)
Cp2-M2-B9	144.4(6)	Cp7-M3-B7	106.2(7)
Cp3-M2-B1	114.1(6)	Cp8-M3-B1	123.2(8)
Cp3-M2-B5	102.3(3)	Cp8-M3-B4	164.1(8)
Cp3-M2-B6	147.0(7)	Cp8-M3-B6	110.1(8)

Table IV. Interatomic Angles (cont'd)

Cp3-M2-B9	106.1(6)	Cp8-M3-B7	142.7(9)
Cp4-M2-B1	154.0(7)	Cp9-M3-B1	97.1(4)
Cp4-M2-B6	108.9(6)	Cp9-M3-B6	145.7(9)
Cp4-M2-B9	92.6(4)	Cp9-M3-B7	154.0(7)
Cp5-M2-B1	150.0(6)	Cp10-M3-B1	106.1(7)
Cp5-M2-B5	158.9(7)	Cp10-M3-B4	104.2(4)
Cp5-M2-B6	97.0(3)	Cp10-M3-B6	157.7(8)
Cp5-M2-B9	115.1(6)	Cp10-M3-B7	116.9(8)

C. Boron-Metal-Boron

B1-M2-B5	49.2(3)	B1-M3-B4	50.1(3)
B1-M2-B6	95.5(3)	B1-M3-B6	95.6(3)
B1-M2-B9	94.4(3)	B1-M3-B7	93.6(3)
B5-M2-B6	85.9(3)	B4-M3-B6	85.7(3)
B5-M2-B9	50.4(3)	B4-M3-B7	48.7(3)
B6-M2-B9	55.1(3)	B6-M3-B7	55.4(3)

D. Boron-Metal-Metal

B1-M2-M3	52.2(2)	B6-M2-M3	54.1(2)
B5-M2-M3	81.2(2)	B9-M2-M3	92.8(2)

E. Carbon-Metal-Metal

Cp1-M2-M3	103.5(3)	Cp4-M2-M3	152.2(6)
Cp2-M2-M3	120.5(4)	Cp5-M2-M3	117.4(5)
Cp3-M2-M3	158.2(7)		

Table IV. Interatomic Angles (cont'd)

## II. B-B-B Angles

B4-B1-B5	63.3(8)	B7-B6-B9	85.6(5)
B1-B4-B5	57.6(4)	B4-B7-B6	101.6(5)
B1-B4-B7	117.6(5)	B4-B7-B8	60.1(5)
B1-B4-B8	113.5(6)	B6-B7-B8	90.0(5)
B5-B4-B7	104.1(6)	B4-B8-B5	61.7(4)
B5-B4-B8	59.5(8)	B4-B8-B7	58.7(5)
B7-B4-B8	61.2(5)	B4-B8-B9	104.7(5)
B1-B5-B4	59.2(4)	B5-B8-B7	103.8(5)
B1-B5-B8	114.5(6)	B5-B8-B9	60.3(5)
B1-B5-B9	117.3(5)	B7-B8-B9	94.8(5)
B4-B5-B8	58.9(5)	B5-B9-B8	59.1(5)
B8-B5-B9	60.6(5)	B6-B9-B8	89.6(5)

## III. C-B-B Angles

C10-B6-B7	52.3(4)	C10-B8-B5	107.2(6)
C10-B6-B9	52.1(4)	C10-B8-B7	55.6(4)
C10-B7-B4	108.3(6)	C10-B8-B9	55.0(4)
C10-B7-B6	51.9(4)	C10-B9-B5	106.9(7)
C10-B7-B8	56.1(5)	C10-B9-B6	52.0(4)
C10-B8-B4	106.7(6)	C10-B9-B8	55.8(4)

## IV. B-C-B Angles

B6-C10-B7	75.8(5)	B7-C10-B8	68.3(5)
B6-C10-B8	112.6(5)	B7-C10-B9	113.0(6)
B6-C10-B9	75.9(4)	B8-C10-B9	69.2(5)

## V. Cyclopentadienyl Ring Angles

Cp2-Cp1-Cp5	109.8(12)	Cp7-Cp6-Cp10	111.0(13)
Cp1-Cp2-Cp3	108.3(10)	Cp6-Cp7-Cp8	104.8(13)
Cp2-Cp3-Cp4	104.4(9)	Cp7-Cp8-Cp9	110.3(13)
Cp3-Cp4-Cp5	108.3(12)	Cp8-Cp9-Cp10	105.3(12)
Cp4-Cp5-Cp1	109.1(12)	Cp9-Cp10-Cp6	108.6(14)

<sup>a</sup>See footnote a of Table I.



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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report 100 ✓	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
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18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Metallocarborane.                      Nickelacarborane. Crystal structure.                      Cobaltacarborane. Bimetallic compound.		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A complete three dimensional crystal structure determination of the title compound was carried out. Crystal data: Space group C2/c, a = 15.794(4), b = 7.955(2), c = 24.273(7) Å, $\beta$ = 104.12(2)°, z = 8, d <sub>0</sub> = 1.55(2), d <sub>c</sub> = 1.54. Diffraction data to 2 $\theta$ <sub>max</sub> = 50° were obtained with a Syntex PT automated diffractometer (MoK $\alpha$ radiation) and the structure was solved by conventional Patterson, Fourier and full matrix least-squares techniques to a conventional R = 0.047 for 2048 independent non-zero reflections. The molecule has the bicapped square antiprismatic geometry expected for a closo ten-vertex polyhedron. The two metal		

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20. (Abstract, cont'd)

atoms are indistinguishable and occupy adjacent sites in the same equatorial belt. The carbon atom resides in the four-coordinate site non-adjacent to the two metal atoms.



**APPENDIX**



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SUPPLEMENTAL MATERIAL

Structure factor amplitudes for 2,3-Di- $\eta$ -cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8)

The table lists the values of h, k, l, cFo and cFc for each observed reflection. The value of c is 2.914.



H	L	FG	FC	H	L	FO	FC	H	L	FO	FC	H	L	PO	PC
****	K	=	0	****											
0	-2	6	88	6	-12	203	201	12	4	131	138	1	6	211	198
0	-2	6	88	6	-10	383	393	12	6	58	60	1	7	170	171
0	-2	6	87	6	-8	133	136	12	8	132	137	1	8	80	79
0	-2	6	87	6	-6	478	472	12	10	79	76	1	9	165	168
0	-2	6	87	6	-4	83	81	12	12	117	123	1	10	240	237
0	-2	6	87	6	-2	336	326	12	14	83	78	1	11	124	123
0	-2	6	87	6	0	65	66	12	16	83	83	1	12	72	73
0	-2	6	87	6	2	481	481	14	-22	118	115	1	13	126	129
0	-2	6	87	6	4	122	126	14	-20	53	53	1	14	191	196
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0	-2	6	87	6	10	241	244	14	-14	132	133	1	17	62	64
0	-2	6	87	6	12	218	220	14	-12	100	102	1	18	131	136
0	-2	6	87	6	14	181	175	14	-10	99	101	1	19	63	69
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0	-2	6	87	8	-28	94	95	14	2	42	43	3	-25	32	33
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0	-2	6	87	8	14	99	104	18	-2	84	87	3	-3	334	338
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5	7	29	29	9	-16	20	10	13	-12	77	82	0	2	69	73
5	8	180	178	9	-14	88	89	13	-11	122	123	0	3	172	167
5	9	199	194	9	-13	62	54	13	-10	111	113	0	4	66	69
5	10	160	163	9	-12	44	50	13	-9	42	38	0	5	398	390
5	11	103	103	9	-11	27	24	13	-8	53	58	0	6	25	35
5	12	139	138	9	-10	108	108	13	-7	100	99	0	7	213	205
5	13	166	165	9	-9	47	42	13	-6	186	188	0	8	23	27
5	14	35	32	9	-8	64	61	13	-5	44	37	0	9	330	325
5	15	76	77	9	-7	32	41	13	-4	61	61	0	10	120	122
5	16	116	112	9	-6	119	114	13	-3	80	79	0	11	138	144
5	17	94	93	9	-5	29	27	13	-2	183	186	0	12	27	36
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5	19	39	47	9	-2	44	41	13	0	30	29	0	14	42	43
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5	21	70	68	9	0	97	94	13	2	129	131	0	17	215	214
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5	24	49	46	9	4	75	79	13	5	76	79	0	21	137	134
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5	30	158	164	11	-26	28	20	13	11	86	82	2	-19	35	29
5	31	120	125	11	-22	49	52	13	12	32	38	2	-17	178	176
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77	77	26	23	77	-9	66	63	11	7	65	68	2	-14	46	53
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77	77	38	38	77	-2	56	57	13	-18	64	60	2	-5	106	106
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H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
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4	11	35	36	6	-1	41	38	8	-7	54	47	10	-2	28	13
6	-	81	81	6	2	100	102	8	-6	57	51				
6	-	29	35	6	3	65	66	8	-5	22	2	***	K =	9	***
6	-	71	70	6	4	33	27	8	-4	23	31	1	-8	37	39
6	-	106	108	6	5	34	29	8	-3	43	40	1	-6	74	68
6	-	26	18	6	6	106	106	8	-2	49	48	1	-4	33	35
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CALIFORNIA UNIV LOS ANGELES DEPT OF CHEMISTRY  
STRUCTURES OF METALLOCARBORANES. IX: CRYSTAL AND MOLECULAR STRU--ETC(U)  
JAN 78 G E HARDY, K P CALLAHAN, M F HAWTHORNE N00014-76-C-0390

F/G 7/2

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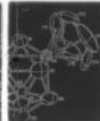
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DEPARTMENT OF CHEMISTRY  
LOS ANGELES, CALIFORNIA 90024

February 24, 1978

TO: Technical Report Distribution List  
FROM: M. F. Hawthorne  
RE: TR's 100 and 101 - corrections, missing page, and missing figure

Please insert the enclosed corrected and missing pages to the technical reports we sent you recently:

The figure goes with TR 100, entitled "Structures of Metallocarboranes. IX. Crystal and Molecular Structure of the Ten-Vertex . . .," by G. E. Hardy, K. P. Callahan, and M. F. Hawthorne. It should be placed behind the last page of Table IV.

Page 15 goes with TR 101, entitled "Synthesis of Closo- and Nido-Metallo-  
cenes," by R. N. Keyden, B. P. Sullivan, R. T. Baker, and M. F. Hawthorne.  
Please replace the old page 15 with this newly corrected copy

Page 25 also goes with TR 101. This reference page was missing from the copy we sent you.

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